

Small polarons in dry DNA

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We report *ab initio* calculations for the hole polaron in dry poly(dC)-poly(dG) DNA. The calculations were performed with the SIESTA method on pieces of DNA from 1 to 4 base pairs, saturated at the ends. Relaxations of the pieces with no charge and with a hole were performed. Our results show clear evidence of self trapping on short lengths giving rise to small polarons. This is supported by different calculated properties, such as the large calculated binding energy (0.30 ± 0.05 eV) and the spatial localization of the hole wavefunction and of the structural deformations. Our estimated activation energy of 0.15 eV for small-polaron hopping compares well with the available experimental value of 0.12 eV.